MPI/OPENMP AFFINITY PERFORMANCE MAPPING AND TESTING

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NATIONAL RENEWABLE ENERGY LABORATORY

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ABSTRACT

The National Renewable Energy Lab has just launched (and submitted a top 500 Run) its newest HPC platform, Kestrel, with 2144 nodes with dual Intel Sapphire Rapids processors.

We'll discuss MPI/OpenMP affinity mapping and testing. We'll present a hybrid MPI/OpenMP test code that reports affinity as a function of environmental settings, tasks, and threads. We show that without attentiveness to affinity, performance can be adversely effected. However, we'll show how to get ideal mapping, where tasks and threads are laid out for performance.

We present a batch script that can be run to sweep over various command line, environmental settings and task/thread combinations. In addition to Intel compilers the script will test Cray, MPICH, and OpenMPI.

We recommend the test code be run before a production run to ensure the desired mappings of tasks and threads. A git repository will be available with all codes and scripts.

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REPO

https://github.com/timkphd/affinity.git

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NREL'S KESTREL ENVIRONMENT

- Slurm
- HPE (Cray) with Slingshot
  - Cray Programming environment - supported by a module system
    - Cray MPI (mpich based)
      - Cray Fortran and C
      - GCC
      - Intel ifort and icc
  - Intel MPI with ifort and icc
  - Others also, but we'll skip for today

CURRENT KESTREL CONFIGURATION

Number of Nodes	Processors	Memory	Accelerators	Local Storage
2144	Dual socket **4th Gen Intel® Xeon® Scalable Processors (52-core)**	256 GB DDR5	N/A	256 nodes with 1.92 TB NVMe M.2
10	Dual socket **4th Gen Intel® Xeon® Scalable Processors (52-core)**	2 TB DDR5	N/A	8 x 1.6 TB NVMe
8	Dual socket **4th Gen Intel® Xeon® Scalable Processors (52-core)**	256 GB DDR5	2 NVIDIA A40 GPUs	2 x 3.84 TB NVMe

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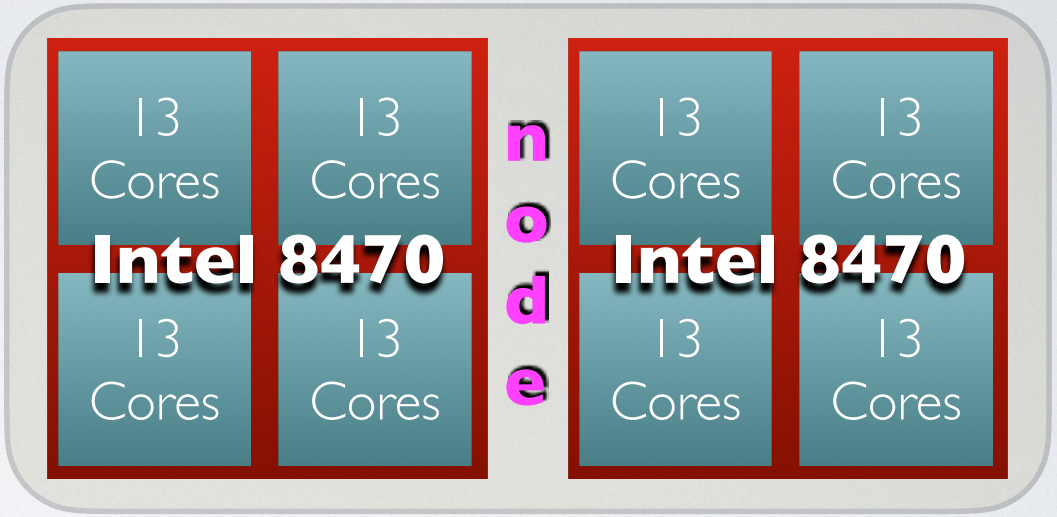
AFFINITY & WHY IMPORTANT

- Affinity - mapping of threads/tasks to cores
- Kestrel 104 cores/node
  - 2 chips (Intel 8470)
    - 52 cores each
    - 4 "tiles" with 13 cores each



- **Worst case: Multiple threads/tasks can end up on the same core potentially reducing performance by 2X or maybe much more**
- Also: You may want to put threads/tasks on particular tiles to maximize communications or memory access
- Possible to have different MPI tasks to have different # threads

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OUR EXAMPLES

- **phostone.c fhostone.F90**
  - Hello world on steroids
  - **Hybrid MPI / OpenMP**
  - Many command line options
  - Will use options to print out a line for each MPI task and OpenMP thread along with the node and core on which it is running: **Show affinity**
  - Will run for 7 seconds.

PHOSTONE.C OUTPUT

```
MPI VERSION Intel(R) MPI Library 2021.10 for Linux* OS
task    thread             node name  first task    # on node  core
0000      0000          X1005C4S5B0N0        0000         0000  0000
0000      0001          X1005C4S5B0N0        0000         0000  0001
0000      0002          X1005C4S5B0N0        0000         0000  0002
0000      0003          X1005C4S5B0N0        0000         0000  0003
0000      0004          X1005C4S5B0N0        0000         0000  0004
0000      0005          X1005C4S5B0N0        0000         0000  0005
0000      0006          X1005C4S5B0N0        0000         0000  0006
0000      0007          X1005C4S5B0N0        0000         0000  0007

0001      0000          X1005C4S5B0N0        0000         0001  0052
0001      0001          X1005C4S5B0N0        0000         0001  0053
0001      0002          X1005C4S5B0N0        0000         0001  0054
0001      0003          X1005C4S5B0N0        0000         0001  0055
0001      0004          X1005C4S5B0N0        0000         0001  0056
0001      0005          X1005C4S5B0N0        0000         0001  0057
0001      0006          X1005C4S5B0N0        0000         0001  0058
0001      0007          X1005C4S5B0N0        0000         0001  0059

0002      0000          X1005c4s6n0n0        0002         0000  0000
0002      0001          X1005c4s6n0n0        0002         0000  0001
0002      0002          X1005c4s6n0n0        0002         0000  0002
0002      0003          X1005c4s6n0n0        0002         0000  0003
0002      0004          X1005c4s6n0n0        0002         0000  0004
0002      0005          X1005c4s6n0n0        0002         0000  0005
0002      0006          X1005c4s6n0n0        0002         0000  0006
0002      0007          X1005c4s6n0n0        0002         0000  0007

0003      0000          X1005c4s6n0n0        0002         0001  0052
0003      0001          X1005c4s6n0n0        0002         0001  0053
0003      0002          X1005c4s6n0n0        0002         0001  0054
0003      0003          X1005c4s6n0n0        0002         0001  0055
0003      0004          X1005c4s6n0n0        0002         0001  0056
0003      0005          X1005c4s6n0n0        0002         0001  0057
0003      0006          X1005c4s6n0n0        0002         0001  0058
0003      0007          X1005c4s6n0n0        0002         0001  0059
total time      7.001
```

- Intel MPI
- 2 nodes
- 2 MPI tasks / node
- 8 OpenMP threads
- Sorted and enhanced

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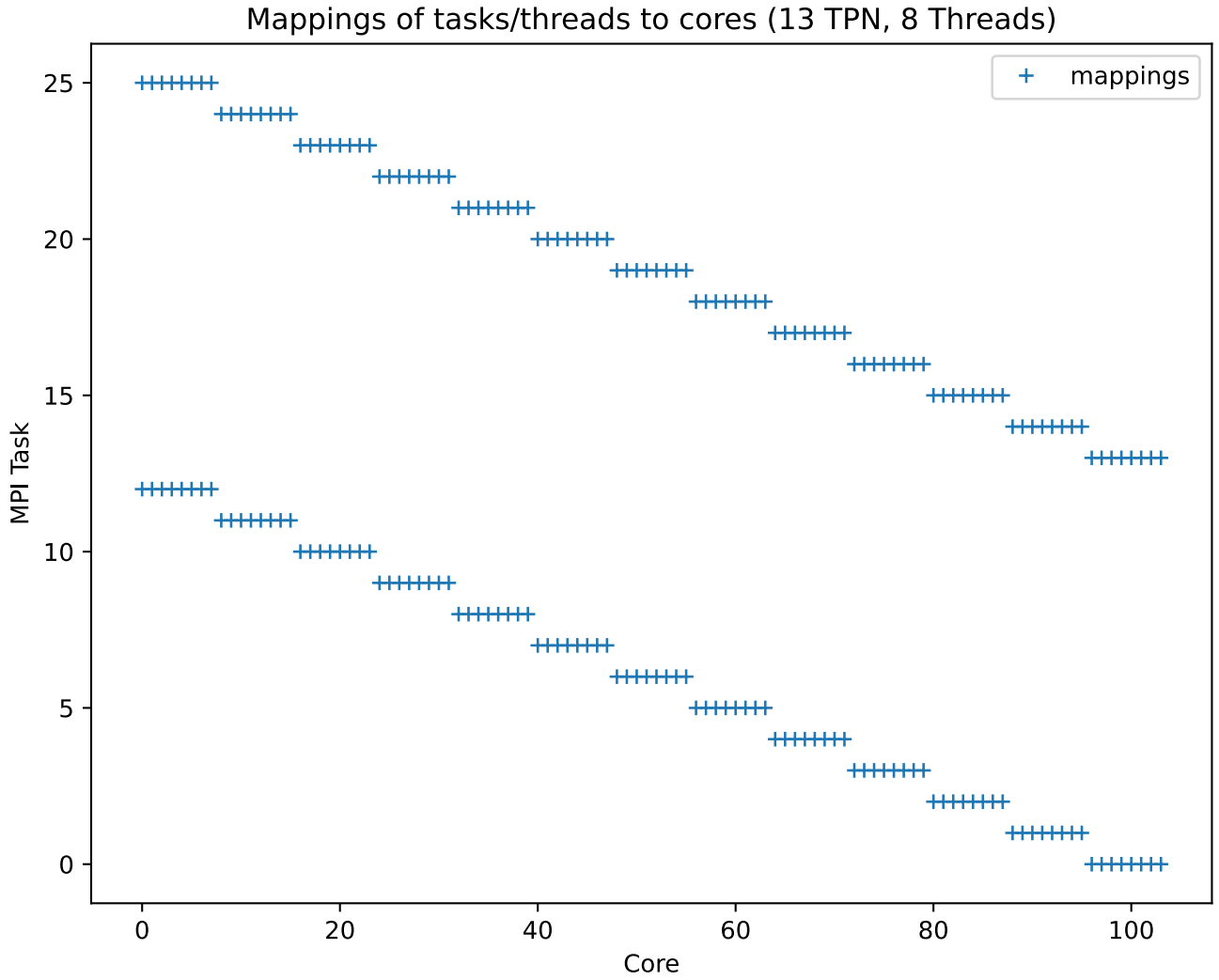
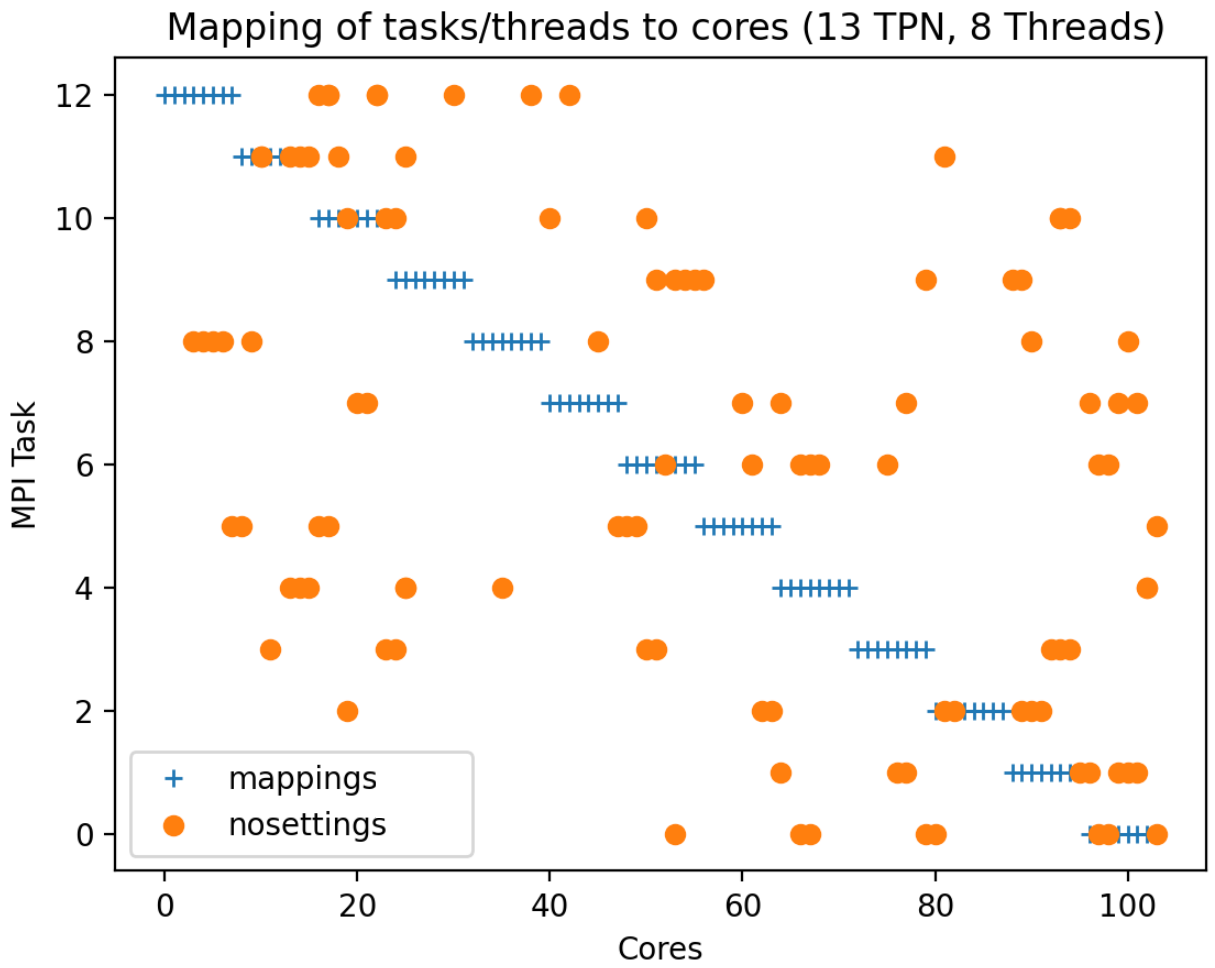
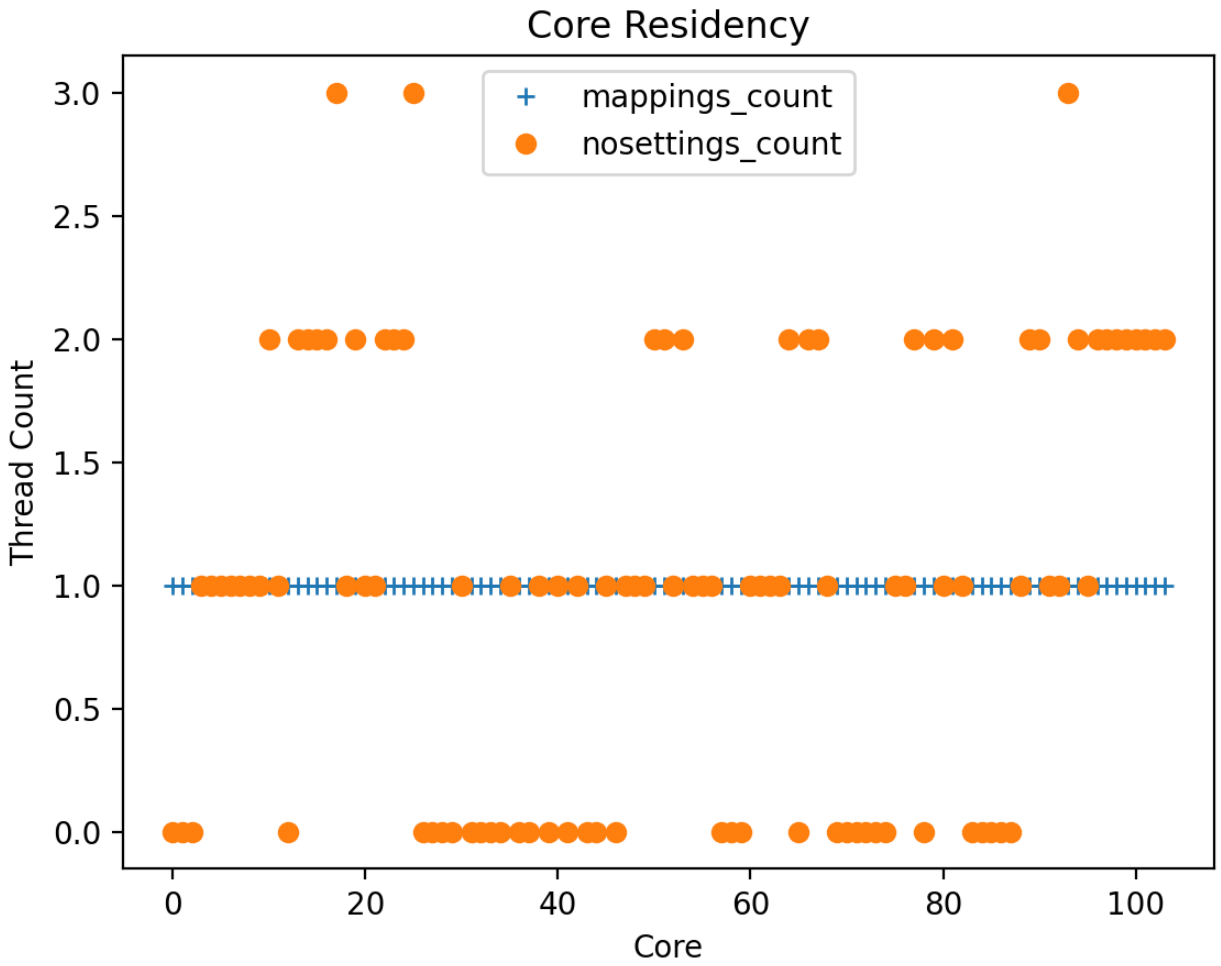
RUN COMMANDS

- Since phostone and fhostone are hybrid MPI/OpenMP codes we will set OpenMP variables.
  - # threads
  - # thread binding
- We'll also add some options to the srun line to tests/ensure we are getting good mapping of tasks and threads to cores
- We can run with various numbers of MPI tasks per node and number of OpenMP threads per task but the two multiplied together should not exceed then number of cores on a node (104).


Mappings of tasks/threads to cores (13 TPN, 8 Threads)
mappings
MPI Task
Core
0
5
10
15
20
25
0
20
40
60
80
100


Mapping of tasks/threads to cores (13 TPN, 8 Threads)
MPI Task
Cores
0
2
4
6
8
10
12
0
20
40
60
80
100
mappings
nosettings


Core Residency
mappings_count
nosettings_count
Thread Count
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
Core

OUR SCRIPT...

- Creates a new directory with "everything"
- Makes all versions of code
- Loops over:
  - Various tasks per node / Threads per task
  - Environment settings and srun command line options
    - Each Compiler/MPI combinations

OUR EXAMPLE SCRIPT

- Reports lots of information
  - Bindings for each run
  - Normal program output for phostrun includes mapping of tasks and threads to nodes and cores
  - MPI launch times
- Final output is a report of successful/failed mapping
  - Success = expected unique combinations of nodes and cores
  - Good News: It works for all tested versions of MPI and mappings (with the correct settings)

CUT TO THE CHASE:

- With the proper setting in sbatch scripts and the srun command we are able to "trivially" get apps to behave reasonably for all cases I tested on Kestrel, Swift and Eagle.
- Masks (a mapping list) allow a fine grain placement of tasks & threads to cores

OVERKILL FOR MOST PEOPLE

- While you can run this for the full set you might not want to use the allocation hours (minutes)
- Suggested use...
  - Run phostone using the exact run arguments you use for your production code to see how it maps tasks and threads to cores

PrgEnv-*

PrgEnv-amd/8.3.3
PrgEnv-aocc/8.3.3
PrgEnv-cray-amd/8.3.3
PrgEnv-cray/8.3.3
PrgEnv-gnu-amd/8.3.3
PrgEnv-gnu/8.3.3
PrgEnv-intel/8.3.3
PrgEnv-nvhpc/8.3.3
PrgEnv-nvidia/8.3.3

- Modules for using Cray's MPI with various backend compilers
- Red one currently work (cray, gnu, intel)
- Blue ones are for AMD processors and Nvidia GPUs (coming)
- PrgEnv-cray/8.3.3 is the default
- **All of these use the same MPI Library (Cray-MPICH)**

"PURE" INTEL SUITE

```
module purge
module load intel-oneapi
module load intel-oneapi-mpi
module load gcc/13.1.0
```

Example Output Intel MPI

```
MPI VERSION Intel(R) MPI Library 2021.10 for Linux* OS

task    thread             node name  first task    # on node  core
0000      0000         X1001C3S0B1N1         0000         0000  0007
0000      0002         X1001C3S0B1N1         0000         0000  0003
0000      0003         X1001C3S0B1N1         0000         0000  0004
0000      0007         X1001C3S0B1N1         0000         0000  0000
0000      0006         X1001C3S0B1N1         0000         0000  0006
0000      0005         X1001C3S0B1N1         0000         0000  0001
0000      0001         X1001C3S0B1N1         0000         0000  0002
0000      0004         X1001C3S0B1N1         0000         0000  0005
0001      0000         X1006C6S0B0N0         0001         0000  0007
0001      0006         X1006C6S0B0N0         0001         0000  0004
0001      0002         X1006C6S0B0N0         0001         0000  0002
0001      0007         X1006C6S0B0N0         0001         0000  0005
0001      0004         X1006C6S0B0N0         0001         0000  0006
0001      0003         X1006C6S0B0N0         0001         0000  0000
0001      0005         X1006C6S0B0N0         0001         0000  0003
0001      0001         X1006C6S0B0N0         0001         0000  0001
mpi_init 0 1698853027.3182 1698853027.8130       0.4949
mpi_init 1 1698853027.3013 1698853027.8136       0.5124
total time      7.004
```

Example Output PrgEnv-*

```
MPI VERSION MPI VERSION    : CRAY MPICH version 8.1.23.5 (ANL base 3.4a2)
MPI BUILD INFO : Tue Nov 29 12:42 2022 (git hash 210ae8b)

task    thread             node name  first task    # on node  core
0000      0001         X1005C2S3B1N1         0000         0000  0001
0000      0003         X1005C2S3B1N1         0000         0000  0003
0000      0005         X1005C2S3B1N1         0000         0000  0005
0000      0004         X1005C2S3B1N1         0000         0000  0004
0000      0006         X1005C2S3B1N1         0000         0000  0006
0000      0000         X1005C2S3B1N1         0000         0000  0000
0000      0002         X1005C2S3B1N1         0000         0000  0002
0000      0007         X1005C2S3B1N1         0000         0000  0007
0001      0000         X1005C3S1B0N0         0001         0000  0000
0001      0002         X1005C3S1B0N0         0001         0000  0002
0001      0001         X1005C3S1B0N0         0001         0000  0001
0001      0006         X1005C3S1B0N0         0001         0000  0006
0001      0004         X1005C3S1B0N0         0001         0000  0004
0001      0005         X1005C3S1B0N0         0001         0000  0005
0001      0007         X1005C3S1B0N0         0001         0000  0007
0001      0003         X1005C3S1B0N0         0001         0000  0003
mpi_init 0 1696732984.4138 1696732984.5317       0.1179
mpi_init 1 1696732984.3726 1696732984.5323       0.1597
total time      7.004
```

makefile

Intel MPI

```
SHELL:=/usr/bin/bash

recurse:
     module purge                       ; \
     module load intel-oneapi           ; \
     module load intel-oneapi-mpi       ; \
     module load gcc/13.1.0             ; \
     $(MAKE) -f $(firstword $(MAKEFILE_LIST)) both

both: f.impi c.impi pp.impi

#defines USEFAST
include makefile.include

ifeq ($(USEFAST),yes)
OPS=-DUSEFAST
EXTRA=getcore.o
endif

F90=mpiifort
CC=mpiicc

f.impi: fhostone.F90 $(EXTRA)
     $(F90) $(OPS) $(EXTRA) -fopenmp fhostone.F90 -O3 -o f.impi
     rm -f getcore.o

c.impi: phostone.c
     $(CC) $(OPS) -fopenmp phostone.c -O3 -o c.impi

pp.impi: ppong.c
     $(CC) $(OPS) $(WES) ppong.c -O3 -o pp.impi

clean:
     rm -rf *o *mod* f.impi c.impi pp.impi
```

- Other makefiles
  - Load different modules
  - Different F90, CC
  - Executable name change
- Makefile - do them all

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```
#!/usr/bin/bash
#SBATCH --job-name="affinity"
#SBATCH --nodes=2
#SBATCH --exclusive
#SBATCH --export=ALL
#SBATCH --time=04:00:00
#SBATCH --partition=standard

BASE=`pwd`

#Make a new directory and go there
STDIR=`pwd`
mkdir $SLURM_JOB_ID
cd $SLURM_JOB_ID

#optionally wait between launches
mywait () { sleep 0; }

#Copy everything
printenv > env
cat $0 > script

cp $BASE/make* .
cp $BASE/Makefile .
cp $BASE/fhostone.F90 .
cp $BASE/phostone.c .
cp $BASE/cases .
cp $BASE/post .
cp $BASE/ppong.c .
cp $BASE/getcore.c .
cp $BASE/maskgenerator.py .
cp $BASE/todo.py .
cp $BASE/tymer  .

tar -czf recreate.tgz *

#Create input for ppong
./todo.py

#Build our programs
make all > make.log 2>&1
make pp  > make.pp 2>&1

#Command line arguments for phostone
CLA="-i -F -E -t 7"
export FEXE=f
export CEXE=c
```

Setup and "make"

make*	Makefiles
Makefile	Driver Makefile
cases	File of tasks and threads
post	Post processing script
maskgenerator.py	Manually creates mapping of threads to cores
todo.py	Creates input file for ppong
tymer	Nice wall clock timer

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Makefile (full)

```
all : impi  cray  gnu  intel open mpich openg mpichg dmod

impi: makeimpi
      make -f makeimpi

cray: makeprgcray
      make -f makeprgcray

gnu: makeprggnu
      make -f makeprggnu

intel: makeprgintel
      make -f makeprgintel

open: makeopen
      make -f makeopen

mpich: makempich
      make -f makempich


openg: makeopen_g
      make -f makeopen_g

mpichg: makempich_g
      make -f makempich_g

clean:
      make -f makeimpi clean
      make -f makeprgintel clean
      make -f makeprggnu clean
      make -f makeprgcray clean
      make -f makeopen clean
      make -f makempich clean
      make -f makeopen_g clean
      make -f makempich_g clean
      rm -rf runall.tgz simple.tgz

dmod:
      rm -rf *.o *mod

pp: pp.impi pp.cray pp.gnu pp.intel pp.open pp.oneapi pp.mpich pp.openg pp.mpichg

pp.impi: makeimpi
      make -f makeimpi pp.impi

pp.cray: makeprgcray
      make -f makeprgcray pp.cray

pp.gnu: makeprggnu
      make -f makeprggnu pp.gnu

pp.intel: makeprgintel
      make -f makeprgintel pp.intel

pp.open: makeopen
      make -f makeopen pp.open

pp.mpich: makempich
      make -f makempich pp.mpich


pp.openg: makeopen_g
      make -f makeopen_g pp.openg

pp.mpichg: makempich_g
      make -f makempich_g pp.mpichg

tar:
      tar -czf runall.tgz \
            cases eagle ecases fhostone.F90 getcore.c make1api Makefile makefile.include \
            makeimpi makeopen makeprgcray makeprggnu makeprgintel maskgenerator.py masks.txt \
            phostone.c post ppong.c readme.md runall runpp subsweep sweep todo.py tymer \
            scases array mapping.py simple makempich makempich_g makeopen_g

simple.tgz:
      tar -czf simple.tgz fhostone.F90  getcore.c  make1api  Makefile  makefile.include  \
           makefile.org  makeimpi  makeopen  makeprgcray  makeprggnu  makeprgintel \
           phostone.c  post  ppong.c simple makempich makempich_g makeopen_g
```

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```
#LOOPING
export CRAY_OMP_CHECK_AFFINITY=TRUE
export nc=`cat cases | wc -l`
for il in `seq $nc` ; do
    aline=`cat cases | head -$il | tail -1`
    ntpn=`echo $aline | awk {'print $1'}`
    nthrd=`echo $aline | awk {'print $2'}`
    export OMP_NUM_THREADS=$nthrd
    for bindit in EMPTY SPREAD THREAD WORKS MASK ; do
        #export KMP_AFFINITY=scatter
        export OMP_PROC_BIND=spread
        export BIND=--cpu-bind=v,${bindit}
        unset CPUS_TASK
        if [ $bindit == MASK ] ; then
        cores=`expr $ntpn \* $nthrd`
        MASK=`./maskgenerator.py $cores $ntpn`
        BIND="--cpu-bind=v,mask_cpu:$MASK"
        fi
        if [ $bindit == NONE ] ; then
        BIND="--cpu-bind=v"
          export CPUS_TASK="--cpus-per-task=$nthrd"
        fi
...
...
        echo $ntpn $nthrd >> srunsettings
        echo $BIND $CPUS_TASK >> srunsettings
        printenv | egrep "OMP_|KMP_" >> srunsettings
        echo --mpi=pmi2 $BIND  --tasks-per-node=$ntpn $CPUS_TASK >> srunsettings
...
...
```

Looping

- Get a task/thread count from each line of cases
- We try various types of thread binding, spread (NONE) and manually (MASK)

- The script maskgenerator.py creates a string describing a mapping of tasks/threads to cores
- This is passed to run using the --cpu-bind option

- Save information for each iteration

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```
./tymer mytimes PrgEnv-intel
          module purge
          module load craype-x86-spr
          module load intel
          module load PrgEnv-intel

./tymer mytimes fortran
          mywait; srun --mpi=pmi2 $BIND  --tasks-per-node=$ntpn $CPUS_TASK  ./$FEXE.intel $CLA > f.intel.out_${ntpn}_${nthrd}_${bindit} \
                 2> f.intel.info_${ntpn}_${nthrd}_${bindit}
./tymer mytimes c
          mywait; srun --mpi=pmi2 $BIND  --tasks-per-node=$ntpn $CPUS_TASK  ./$CEXE.intel $CLA > c.intel.out_${ntpn}_${nthrd}_${bindit} \
                 2> c.intel.info_${ntpn}_${nthrd}_${bindit}
./tymer mytimes finished

          if [[ $nthrd -eq 1 &&  $ntpn -eq 104 && $bindit == NONE ]] ; then
          mywait; srun --mpi=pmi2 $BIND  --tasks-per-node=$ntpn $CPUS_TASK  ./pp.intel $CLA > pp.intel.xxx_${ntpn}_${nthrd}_${bindit} \
                                  2> pp.intel.iii_${ntpn}_${nthrd}_${bindit}
./tymer mytimes finished ppong
          fi

./tymer mytimes PrgEnv-gnu
          module purge
          module load craype-x86-spr
          module load PrgEnv-gnu

./tymer mytimes fortran
          mywait; srun --mpi=pmi2 $BIND  --tasks-per-node=$ntpn $CPUS_TASK  ./$FEXE.gnu $CLA > f.gnu.out_${ntpn}_${nthrd}_${bindit} \
                 2> f.gnu.info_${ntpn}_${nthrd}_${bindit}
./tymer mytimes c
          mywait; srun --mpi=pmi2 $BIND  --tasks-per-node=$ntpn $CPUS_TASK  ./$CEXE.gnu $CLA > c.gnu.out_${ntpn}_${nthrd}_${bindit} \
                 2> c.gnu.info_${ntpn}_${nthrd}_${bindit}
./tymer mytimes finished

          if [[ $nthrd -eq 1 &&  $ntpn -eq 104 && $bindit == NONE ]] ; then
          mywait; srun --mpi=pmi2 $BIND  --tasks-per-node=$ntpn $CPUS_TASK  ./pp.gnu $CLA > pp.gnu.xxx_${ntpn}_${nthrd}_${bindit} \
                                  2> pp.gnu.iii_${ntpn}_${nthrd}_${bindit}
./tymer mytimes finished ppong
          fi
```

```
./tymer mytimes PrgEnv-cray
    module purge
    module load craype-x86-spr
    module load PrgEnv-cray

./tymer mytimes fortran
    mywait; srun --mpi=pmi2 $BIND  --tasks-per-node=$ntpn $CPUS_TASK  ./$FEXE.cray $CLA > f.cray.out_${ntpn}_${nthrd}_${bindit} \
        2> f.cray.info_${ntpn}_${nthrd}_${bindit}
./tymer mytimes c
    mywait; srun --mpi=pmi2 $BIND  --tasks-per-node=$ntpn $CPUS_TASK  ./$CEXE.cray $CLA > c.cray.out_${ntpn}_${nthrd}_${bindit} \
        2> c.cray.info_${ntpn}_${nthrd}_${bindit}
./tymer mytimes finished

    if [[ $nthrd -eq 1 &&  $ntpn -eq 104 && $bindit == NONE ]] ; then
    mywait; srun --mpi=pmi2 $BIND  --tasks-per-node=$ntpn $CPUS_TASK  ./pp.cray $CLA > pp.cray.xxx_${ntpn}_${nthrd}_${bindit} \
              2> pp.cray.iii_${ntpn}_${nthrd}_${bindit}
./tymer mytimes finished ppong
    fi

./tymer mytimes intel-oneapi
    module purge
    module load intel-oneapi
    module load libfabric

./tymer mytimes fortran
    mywait; srun --mpi=pmi2 $BIND  --tasks-per-node=$ntpn $CPUS_TASK  ./$FEXE.impi $CLA > f.impi.out_${ntpn}_${nthrd}_${bindit} \
        2> f.impi.info_${ntpn}_${nthrd}_${bindit}
./tymer mytimes c
    mywait; srun --mpi=pmi2 $BIND  --tasks-per-node=$ntpn $CPUS_TASK  ./$CEXE.impi $CLA > c.impi.out_${ntpn}_${nthrd}_${bindit} \
        2> c.impi.info_${ntpn}_${nthrd}_${bindit}
./tymer mytimes finished

    if [[ $nthrd -eq 1 &&  $ntpn -eq 104 && $bindit == NONE ]] ; then
    mywait; srun --mpi=pmi2 $BIND  --tasks-per-node=$ntpn $CPUS_TASK  ./pp.impi $CLA > pp.impi.xxx_${ntpn}_${nthrd}_${bindit} \
              2> pp.impi.iii_${ntpn}_${nthrd}_${bindit}
./tymer mytimes finished ppong
    fi
   done
done
```

```
./post
. ./post | sort -n > posit
getstate postit nope > report
getstate postit worked >> report
mv $STDIR/slurm-$SLURM_JOB_ID.out .
```

Post processing

- Report of successful and failed phostone runs
- Copy slurm output to our final directory
- Might want to look at output from ppong
  - Bandwidth
  - MPI_Barrier rate
- Might want to look at MPI_Init times from phostone

REPORT

```
tkaiser2-37907s:177402 tkaiser2$ cat report
c.cray.out_104_1_MASK 208 208
c.cray.out_104_1_NONE 208 208
c.cray.out_1_104_MASK 208 208
c.cray.out_1_104_NONE 208 208
c.cray.out_1_8_MASK 16 16
c.cray.out_1_8_NONE 16 16
c.gnu.out_104_1_MASK 208 208
c.gnu.out_104_1_NONE 208 208
c.gnu.out_1_104_MASK 208 208
c.gnu.out_1_104_NONE 208 208
c.gnu.out_1_8_MASK 16 16
c.gnu.out_1_8_NONE 16 16
c.impi.out_104_1_MASK 208 208
c.impi.out_104_1_NONE 208 208
c.impi.out_1_104_MASK 208 208
c.impi.out_1_104_NONE 208 208
c.impi.out_1_8_MASK 16 16
c.impi.out_1_8_NONE 16 16
c.intel.out_104_1_MASK 208 208
c.intel.out_104_1_NONE 208 208
c.intel.out_1_104_MASK 208 208
c.intel.out_1_104_NONE 208 208
c.intel.out_1_8_MASK 16 16
c.intel.out_1_8_NONE 16 16
```

```
f.cray.out_104_1_MASK 208 208
f.cray.out_104_1_NONE 208 208
f.cray.out_1_104_MASK 208 208
f.cray.out_1_104_NONE 208 208
f.cray.out_1_8_MASK 16 16
f.cray.out_1_8_NONE 16 16
f.gnu.out_104_1_MASK 208 208
f.gnu.out_104_1_NONE 208 208
f.gnu.out_1_104_MASK 208 208
f.gnu.out_1_104_NONE 208 208
f.gnu.out_1_8_MASK 16 16
f.gnu.out_1_8_NONE 16 16
f.impi.out_104_1_MASK 208 208
f.impi.out_104_1_NONE 208 208
f.impi.out_1_104_MASK 208 208
f.impi.out_1_104_NONE 208 208
f.impi.out_1_8_MASK 16 16
f.impi.out_1_8_NONE 16 16
f.intel.out_104_1_MASK 208 208
f.intel.out_104_1_NONE 208 208
f.intel.out_1_104_MASK 208 208
f.intel.out_1_104_NONE 208 208
f.intel.out_1_8_MASK 16 16
f.intel.out_1_8_NONE 16 16
```

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RUN SETTINGS

AS NAMED IN THE SCRIPT

EMPTY

- export OMP_NUM_THREADS=$nthrd
- --cpu-bind=v

SPREAD

- export OMP_NUM_THREADS=$nthrd
- export OMP_PROC_BIND=spread
- --cpu-bind=v

THREAD

- export OMP_NUM_THREADS=$nthrd
- --cpu-bind=v
- --cpus-per-task=$nthrd

WORKS

- export OMP_NUM_THREADS=$nthrd
- export OMP_PROC_BIND=spread
- --cpu-bind=v
- --cpus-per-task=$nthrd

MASK

- export OMP_NUM_THREADS=$nthrd
- export OMP_PROC_BIND=spread
- --cpu-bind=v,mask_cpu:$MASK

EMPTY

Language	MPI	Tasks	Threads	Expected Cores	Cores Used	Status
C,Cray	Cray	104	1	208	208	
C,gnu	Cray	104	1	208	208	
C,Intel	INTEL	104	1	208	208	
C,Intel	Cray	104	1	208	208	
Fortran,Cray	Cray	104	1	208	208	
Fortran,gnu	Cray	104	1	208	208	
ifort	INTEL	104	1	208	208	
ifort	Cray	104	1	208	208	
C,Cray	Cray	1	104	208	208	
C,gnu	Cray	1	104	208	208	
C,Intel	INTEL	1	104	208	153	Failed
C,Intel	Cray	1	104	208	152	Failed
Fortran,Cray	Cray	1	104	208	208	
Fortran,gnu	Cray	1	104	208	208	
ifort	INTEL	1	104	208	103	Failed
ifort	Cray	1	104	208	96	Failed
C,Cray	Cray	13	8	208	208	
C,gnu	Cray	13	8	208	208	
C,Intel	INTEL	13	8	208	207	Failed
C,Intel	Cray	13	8	208	208	
Fortran,Cray	Cray	13	8	208	106	Failed
Fortran,gnu	Cray	13	8	208	107	Failed
ifort	INTEL	13	8	208	143	Failed
ifort	Cray	13	8	208	137	Failed

Language	MPI	Tasks	Threads	Expected Cores	Cores Used	Status
C,Cray	Cray	1	8	16	16	
C,gnu	Cray	1	8	16	16	
C,Intel	INTEL	1	8	16	16	
C,Intel	Cray	1	8	16	16	
Fortran,Cray	Cray	1	8	16	16	
Fortran,gnu	Cray	1	8	16	16	
ifort	INTEL	1	8	16	16	
ifort	Cray	1	8	16	16	
C,Cray	Cray	8	13	208	208	
C,gnu	Cray	8	13	208	208	
C,Intel	INTEL	8	13	208	208	
C,Intel	Cray	8	13	208	208	
Fortran,Cray	Cray	8	13	208	111	Failed
Fortran,gnu	Cray	8	13	208	107	Failed
ifort	INTEL	8	13	208	150	Failed
ifort	Cray	8	13	208	164	Failed

- export OMP_NUM_THREADS=$nthrd
- --cpu-bind=v

SPREAD

Language	MPI	Tasks	Threads	Expected Cores	Cores Used	Status
C,Cray	Cray	104	1	208	208	
C,gnu	Cray	104	1	208	208	
C,Intel	INTEL	104	1	208	208	
C,Intel	Cray	104	1	208	208	
Fortran,Cray	Cray	104	1	208	208	
Fortran,gnu	Cray	104	1	208	208	
ifort	INTEL	104	1	208	208	
ifort	Cray	104	1	208	208	
C,Cray	Cray	1	104	208	208	
C,gnu	Cray	1	104	208	208	
C,Intel	INTEL	1	104	208	208	
C,Intel	Cray	1	104	208	208	
Fortran,Cray	Cray	1	104	208	208	
Fortran,gnu	Cray	1	104	208	208	
ifort	INTEL	1	104	208	208	
ifort	Cray	1	104	208	208	
C,Cray	Cray	13	8	208	16	Failed
C,gnu	Cray	13	8	208	16	Failed
C,Intel	INTEL	13	8	208	16	Failed
C,Intel	Cray	13	8	208	16	Failed
Fortran,Cray	Cray	13	8	208	16	Failed
Fortran,gnu	Cray	13	8	208	16	Failed
ifort	INTEL	13	8	208	16	Failed
ifort	Cray	13	8	208	16	Failed

Language	MPI	Tasks	Threads	Expected Cores	Cores Used	Status
C,Cray	Cray	1	8	16	16	
C,gnu	Cray	1	8	16	16	
C,Intel	INTEL	1	8	16	16	
C,Intel	Cray	1	8	16	16	
Fortran,Cray	Cray	1	8	16	16	
Fortran,gnu	Cray	1	8	16	16	
ifort	INTEL	1	8	16	16	
ifort	Cray	1	8	16	16	
C,Cray	Cray	8	13	208	26	Failed
C,gnu	Cray	8	13	208	26	Failed
C,Intel	INTEL	8	13	208	26	Failed
C,Intel	Cray	8	13	208	26	Failed
Fortran,Cray	Cray	8	13	208	26	Failed
Fortran,gnu	Cray	8	13	208	26	Failed
ifort	INTEL	8	13	208	26	Failed
ifort	Cray	8	13	208	26	Failed

- export OMP_NUM_THREADS=$nthrd
- export OMP_PROC_BIND=spread
- --cpu-bind=v

THREAD

Language	MPI	Tasks	Threads	Expected Cores	Cores Used	Status
C,Cray	Cray	104	1	208	208	
C,gnu	Cray	104	1	208	208	
C,Intel	INTEL	104	1	208	208	
C,Intel	Cray	104	1	208	208	
Fortran,Cray	Cray	104	1	208	208	
Fortran,gnu	Cray	104	1	208	208	
ifort	INTEL	104	1	208	208	
ifort	Cray	104	1	208	208	
C,Cray	Cray	1	104	208	208	
C,gnu	Cray	1	104	208	208	
C,Intel	INTEL	1	104	208	155	
C,Intel	Cray	1	104	208	167	
Fortran,Cray	Cray	1	104	208	208	
Fortran,gnu	Cray	1	104	208	208	
ifort	INTEL	1	104	208	98	Failed
ifort	Cray	1	104	208	96	Failed
C,Cray	Cray	13	8	208	208	
C,gnu	Cray	13	8	208	208	
C,Intel	INTEL	13	8	208	206	Failed
C,Intel	Cray	13	8	208	205	Failed
Fortran,Cray	Cray	13	8	208	208	
Fortran,gnu	Cray	13	8	208	208	
ifort	INTEL	13	8	208	155	Failed
ifort	Cray	13	8	208	155	Failed

Language	MPI	Tasks	Threads	Expected Cores	Cores Used	Status
C,Cray	Cray	1	8	16	16	
C,gnu	Cray	1	8	16	16	
C,Intel	INTEL	1	8	16	16	
C,Intel	Cray	1	8	16	16	
Fortran,Cray	Cray	1	8	16	16	
Fortran,gnu	Cray	1	8	16	16	
ifort	INTEL	1	8	16	16	
ifort	Cray	1	8	16	16	
C,Cray	Cray	8	13	208	208	
C,gnu	Cray	8	13	208	208	
C,Intel	INTEL	8	13	208	208	
C,Intel	Cray	8	13	208	208	
Fortran,Cray	Cray	8	13	208	208	
Fortran,gnu	Cray	8	13	208	208	
ifort	INTEL	8	13	208	208	
ifort	Cray	8	13	208	208	

- export OMP_NUM_THREADS=$nthrd
- --cpu-bind=v
- --cpus-per-task=$nthrd
- *--threads-per-core=1*

WORKS

Language	MPI	Tasks	Threads	Expected Cores	Cores Used	Status
C,Cray	Cray	104	1	208	208	
C,gnu	Cray	104	1	208	208	
C,Intel	INTEL	104	1	208	208	
C,Intel	Cray	104	1	208	208	
Fortran,Cray	Cray	104	1	208	208	
Fortran,gnu	Cray	104	1	208	208	
ifort	INTEL	104	1	208	208	
ifort	Cray	104	1	208	208	
C,Cray	Cray	1	104	208	208	
C,gnu	Cray	1	104	208	208	
C,Intel	INTEL	1	104	208	208	
C,Intel	Cray	1	104	208	208	
Fortran,Cray	Cray	1	104	208	208	
Fortran,gnu	Cray	1	104	208	208	
ifort	INTEL	1	104	208	208	
ifort	Cray	1	104	208	208	
C,Cray	Cray	13	8	208	208	
C,gnu	Cray	13	8	208	208	
C,Intel	INTEL	13	8	208	208	
C,Intel	Cray	13	8	208	208	
Fortran,Cray	Cray	13	8	208	208	
Fortran,gnu	Cray	13	8	208	208	
ifort	INTEL	13	8	208	208	
ifort	Cray	13	8	208	208	

Language	MPI	Tasks	Threads	Expected Cores	Cores Used	Status
C,Cray	Cray	1	8	16	16	
C,gnu	Cray	1	8	16	16	
C,Intel	INTEL	1	8	16	16	
C,Intel	Cray	1	8	16	16	
Fortran,Cray	Cray	1	8	16	16	
Fortran,gnu	Cray	1	8	16	16	
ifort	INTEL	1	8	16	16	
ifort	Cray	1	8	16	16	
C,Cray	Cray	8	13	208	208	
C,gnu	Cray	8	13	208	208	
C,Intel	INTEL	8	13	208	208	
C,Intel	Cray	8	13	208	208	
Fortran,Cray	Cray	8	13	208	208	
Fortran,gnu	Cray	8	13	208	208	
ifort	INTEL	8	13	208	208	
ifort	Cray	8	13	208	208	

- export OMP_NUM_THREADS=$nthrd
- export OMP_PROC_BIND=spread
- --cpu-bind=v
- --cpus-per-task=$nthrd

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MASK

Language	MPI	Tasks	Threads	Expected Cores	Cores Used	Status
C,Cray	Cray	104	1	208	208	
C,gnu	Cray	104	1	208	208	
C,Intel	INTEL	104	1	208	208	
C,Intel	Cray	104	1	208	208	
Fortran,Cray	Cray	104	1	208	208	
Fortran,gnu	Cray	104	1	208	208	
ifort	INTEL	104	1	208	208	
ifort	Cray	104	1	208	208	
C,Cray	Cray	1	104	208	208	
C,gnu	Cray	1	104	208	208	
C,Intel	INTEL	1	104	208	208	
C,Intel	Cray	1	104	208	208	
Fortran,Cray	Cray	1	104	208	208	
Fortran,gnu	Cray	1	104	208	208	
ifort	INTEL	1	104	208	208	
ifort	Cray	1	104	208	208	
C,Cray	Cray	13	8	208	208	
C,gnu	Cray	13	8	208	208	
C,Intel	INTEL	13	8	208	208	
C,Intel	Cray	13	8	208	208	
Fortran,Cray	Cray	13	8	208	208	
Fortran,gnu	Cray	13	8	208	208	
ifort	INTEL	13	8	208	208	
ifort	Cray	13	8	208	208	

WORKS-1

Language	MPI	Tasks	Threads	Expected Cores	Cores Used	Status
C,Cray	Cray	1	8	16	16	
C,gnu	Cray	1	8	16	16	
C,Intel	INTEL	1	8	16	16	
C,Intel	Cray	1	8	16	16	
Fortran,Cray	Cray	1	8	16	16	
Fortran,gnu	Cray	1	8	16	16	
ifort	INTEL	1	8	16	16	
ifort	Cray	1	8	16	16	
C,Cray	Cray	8	13	208	208	
C,gnu	Cray	8	13	208	208	
C,Intel	INTEL	8	13	208	208	
C,Intel	Cray	8	13	208	208	
Fortran,Cray	Cray	8	13	208	208	
Fortran,gnu	Cray	8	13	208	208	
ifort	INTEL	8	13	208	208	
ifort	Cray	8	13	208	208	

- export OMP_NUM_THREADS=$nthrd
- export OMP_PROC_BIND=spread
- --cpu-bind=v,mask_cpu:$MASK

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ABOUT MASKS

- Masks are specified as a string with N task values
- Each value gives the cores on which MPI task N-1 can reside
- Masks are either Decimal or Hex but are interpreted as binary
- Does not guarantee threads will be even distributed between allowed cores

```
mask=0xfff80000000000000000000,0x7ffc0000000000000000,0x3ffe0000000000000,0x1fff00000000000,0xfff8000000000,
0x7ffc000000,0x3ffe000,0x1fff
>>> for task in range(0,8) :
...     print(task, f'{input[task]:0104b}')
...
0 1111111111111000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000
1 0000000000001111111111111000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000
2 0000000000000000000000001111111111111000000000000000000000000000000000000000000000000000000000000000000000000000000000000000
3 0000000000000000000000000000000001111111111111000000000000000000000000000000000000000000000000000000000000000000000000000000
4 0000000000000000000000000000000000000000000001111111111111000000000000000000000000000000000000000000000000000000000000000000
5 0000000000000000000000000000000000000000000000000000000001111111111111000000000000000000000000000000000000000000000000000000
6 0000000000000000000000000000000000000000000000000000000000000000000001111111111111000000000000000000000000000000000000000000
7 0000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000
>>>
```

8 Tasks, 13 threads

RECOMMENDATIONS

- Download the repo
  - Change module loads to match you system
  - Run it
- Build phostone with your environment
- Run with your srun and env settings to see that you have proper mappings
  - May want to add --threads-per-core=1 to your srun line
- **Don't rely on "default" settings and assume you have good affinity**

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REPO AND CONTACT

https://github.com/timkphd/affinity.git

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